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The X-ray Beam and Biological Crystal Visualization for Macromolecular Crystallography

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The SBC on-axis visualization system allows viewing of x-ray beam and biological crystals from x-ray beam direction without parallax distortion. The system was constructed using non-dispersive optics: a long-working-distance Maksutov–Cassagrain reflective microscope and right-angle (45º) mirror. This on-axis geometry allows crystal visualization during diffraction data collection with full Kappa geometry.

An x-ray beam and biological crystal imaging system during data collection has been developed. The direct x-ray beam uses x-ray excited ultraviolet (UV) fluorescence. The high-energy radiation such as x-ray and middle UV (MUV) radiation excite "visible" light luminescence from biological materials, which can be imaged with CCD cameras. The fluorescence from biological crystals is primarily emitted as near-UV (NUV) wavelengths between 300–360 nm depending on the biological material and surrounding environment. We demonstrate detection of biological crystal location using x-ray excited UV fluorescence. We discuss techniques for biological crystal location using intrinsic x-ray excited and MUV excited UV fluorescence from biological crystals.

The x-ray beam can be characterized using a scintillator (phosphor or a single crystal) that converts x-ray photons into visible light photons, which can be imaged using SBC on-axis optics. The x-ray penetration is dependent on the composition of the scintillator (especially effective Z) and x-ray energy. Several scintillators have been used to visualize x-ray beams. Here we compare $CdWO_4$, $PbWO_4$, $Bi_4Ge_3O_{12}$, $Y_3Al_5O_{12}$:Ce (YAG), and Gd_2O_2S:Tb (phosphor). The synchrotron x-ray beam profile studies were done using on-axis and off on-axis imaging. We determined that scintillators made of $CdWO_4$ and similar high-Z single-crystal materials are best suited for the energy range (7–20 keV) and are most suitable for beam visualization for macromolecular crystallography applications. These scintillators show excellent absorption, optical, and mechanical properties.

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